IMPORTANT NOTICE: The current official version of this document is available via the Sandia National Laboratories WIPP On-line Documents web site. A printed copy of this document may not be the version currently in effect.

Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Plan for Modifying Parameter Distributions for S_MB139:COMP_RCK and S_MB139:SAT_RGAS

AP-118

Task number
1.2.7

Effective Date: 02/03/05

Author:	Eric Vugrin (6821)	*Original signed by Eric D. Vugrin*	*2/2/05*
	Print	Signature	Date

Author:	Thomas Kirchner (6821)	*Original signed by Thomas Kirchner*	*2/2/05*
	Print	Signature	Date

Technical
Review:	Martin Nemer (6821)	*Original signed by Martin Nemer*	*2/2/05*
	Print	Signature	Date

Management
Review:	David Kessel (6821)	*Original signed by David Kessel*	*2/3/05*
	Print	Signature	Date

QA
Review:	Mario Chavez (6820)	*Original signed by Mario Chavez*	*2/3/05*
	Print	Signature	Date

<u>TABLE OF CONTENTS</u>

1 INTRODUCTION AND OBJECTIVES

In March of 2004, Sandia National Laboratories completed a Performance Assessment of the Waste Isolation Pilot Plant (WIPP) for the Compliance Recertification Application (CRA) (U.S. DOE 2004). Both subjective and stochastic uncertainty are considered by the WIPP PA. Subjective uncertainty concerns the uncertainty of the values of various model parameters, and WIPP PA models use approximately seventy uncertain parameters.

To account for this uncertainty, the WIPP PA uses Latin hypercube sampling which ensures that sampled values are independent and that the extremes of each parameter's range are represented in the results. The 2004 WIPP PA used the code LHS version 2.41 to perform the Latin hypercube sampling (WIPP-PA 2004). Hansen (2004) identified that the code was incorrectly sampling from the truncated normal and lognormal distributions. (It should be noted that this error does not impact any CRA calculations since no sampled parameters used normal or lognormal distributions for the CRA.) Additionally, for uniformity, it was determined that student and logstudent parameters would be sampled from ranges bounded by the 1st and 99th quantiles (Vugrin 2005). These are the same quantiles used for normal and lognormal distributions.

This change in sampling methodology for parameters modeled with student and logstudent distributions can lead to some physically unrealistic sampled values. Most notably, sampled values of the parameters S_MB139:COMP_RCK and S_MB139:SAT_RGAS should be restricted between 0.00 and 1.00 so that they represent physically realistic values, but when these parameters are modeled with student distributions, their first quantiles correspond to negative values. (These parameters are used by the code BRAGFLO, the WIPP PA code that simulates gas and brine flow as well as incorporating the effects of disposal room consolidation and closure, gas generation, and interbed fracture in response to gas pressure (WIPP-PA 2003)).

The objective of this analysis is to analyze the parameters S_MB139:COMP_RCK and S_MB139:SAT_RGAS and determine if the distributions with which they are modeled are appropriate. In addition, a sensitivity analysis will be conducted to determine if BRAGFLO is truly sensitive to the model parameters. This analysis will determine if

1) the parameters should be modeled with different distributions than the ones that are currently used to model them,
2) the models that use the parameters are insensitive to those parameters, and the parameters can be set to a constant for future calculations, or
3) the parameters' distributions should remain unchanged.

2   APPROACH

For each parameter to be analyzed, five to ten different values will be selected to encompass a broad range of values currently allowed for sampling. Several BRAGFLO vectors from the 2004 CRA will be screened out for comparison based upon the magnitude of their mean direct brine releases (DBRs). For each selected vector, BRAGFLO will be executed for scenarios S1 and S2 for each selected value of the parameter that is being analyzed. All other parameter inputs for that execution of BRAGFLO will remain the same as were used in the CRA. For each set of parameter values, BRAGFLO outputs (such as repository pressure and brine saturation levels) will be compared for each scenario/vector combination. Based upon these sensitivity analyses, it will be determined if the outputs of the BRAGFLO model are truly sensitive to its input parameters. If the code is deemed insensitive to the parameter, the parameter will be assigned a constant value to be determined by the code sponsor.

If the code is determined to be sensitive to the parameter under review, Monte Carlo analysis and other techniques will be used to determine a distribution that is appropriate for the parameter. Commercial off-the-shelf software (COTS), such as Crystal Ball®, may be used to for this analysis.

3   SOFTWARE LIST

For the parameter review, BRAGFLO version 5.00 will be used. Calculations will be performed on the WIPP PA Alpha Cluster. Additionally, COTS software, such as Crystal Ball®, Excel®, and Access®, may be used in this analysis.

4   TASKS

The schedule, tasks, and responsible individuals are outlined in Table 1.

Table 1 Parameter Review: Tasks and Responsibilities

Estimated Date of Completion	Task(s)	Responsible Individual
March 1, 2005	Prepare input files	William Zelinski
April 1, 2005	BRAGFLO Calculations	Bart Buell Jennifer Long
June 1, 2005	Analysis of Results	Thomas Kirchner Joshua Stein Eric Vugrin William Zelinski

5   SPECIAL CONSIDERATIONS

None.

6   APPLICABLE PROCEDURES

Analyses will be conducted in accordance with the quality assurance (QA) procedures listed below.

Training: Training will be performed in accordance with the requirements in NP 2-1.

Parameter Development and Database Management: Selection and documentation of parameter values will follow NP 9-2. The database will be managed in accordance with relevant technical procedure.

Computer Codes: All computer codes that will be used in the analyses will be qualified in accordance with NP 19-1. Codes will be run on the WIPP PA Alpha cluster running Open VMS Version 7.3-1

Analysis and Documentation: Documentation will meet the applicable requirements in NP 9-1.

Reviews: Reviews will be conducted and documented in accordance with NP 6-1 and NP 9-1, as appropriate.

7   REFERENCES

Hansen, C. 2004. Software Problem Report. Sandia National Laboratories. Carlsbad, NM. ERMS #535667.

U.S. DOE. 2004. Title 40 CFR Part 191 Compliance Recertification Application for the Waste Isolation Pilot. DOE/WIPP 2004-3231, U.S. Department of Energy Waste Isolation Pilot Plant, Carlsbad Field Office, Carlsbad, NM.

Vugrin, E. 2005. Change Control Form for LHS version 2.41 to LHS version 2.42. Sandia National Laboratories. Carlsbad, NM. ERMS# 538375.

WIPP-PA (Performance Assessment) (2004). User's Manual for LHS Version 2.41. Sandia National Laboratories. Carlsbad, NM. ERMS# 230732.

WIPP-PA (Performance Assessment) (2003). User's Manual for BRAGFLO Version 5.00. Sandia National Laboratories. Carlsbad, NM. ERMS# 525702.